=> d his

```
(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)
     FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001
                STRUCTURE UPLOADED
L1
              1 S L
L2
L3
            477 S L2 FULL
     FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001
L4
            133 S L3
L5
                STRUCTURE
                          UPLOADED
                S L5
     FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001
L6
              1 S L5
     FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001
L7
              1 S L6
     FILE 'REGISTRY' ENTERED AT 20:5%:35 ON 17 JUN 2001
            459 S L5/ FULL
^{18}
            459 S LA FULL
L9
     FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001
                STRUCTURE UPLOADED
L10
              0 $\mathbb{f} L10
L11
              1 /S L11 FULL
L12
     FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 200
L13
               2 S L12
L14
              1 S L13 AND BERNARDON, J?/AU
              1 S L13 NOT L14
L15
              0 S L15 AND PD < JULY 1998
L16
     FILE 'REGISTRY' ENTERED AT 21:03:39 ON 17 JUN 2001
                STRUCTURE UPLOADED
L17
              0 S L17
L18
              0 S L18 FULL
L19
L20
                STRUCTURE UPLOADED
              0 S L20
L21
L22
              6 S L21 FULL
     FILE 'HCAPLUS' ENTERED AT 21:05:16 ON 17 JUN 2001
L23
             16 S L22
L24
              1 S L23 AND BERNARDON, J?/AU
L25
              7 S L23 AND PD < JULY 1998
     FILE 'CAOLD' ENTERED AT 21:06:44 ON 17 JUN 2001
=> s 122
L26
            0 L22
```

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
|--|------------|---------|
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.31 | 851.81 |
| | | • |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -5.26 |
| | | |

STN INTERNATIONAL LOGOFF AT 21:06:59 ON 17 JUN 2001

```
соон
chain nodes :
   11 14 15
ring nodes :
   1 2 3 4 5 6 7 8 9 10
chain bonds :
   11-14 14-15
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
   11-14 14-15
exact bonds :
   1-2 1-6 2-3 3-4 4-5
normalized bonds :
   5-6 5-7 6-10 7-8 8-9 9-10
isolated ring systems :
   containing 1 :
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS

: Unsaturated

 \sim

Match level :

14:

Generic attributes :

Saturation

12:CLASS 14:Atom 15:CLASS

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

1

STN Structure : 9719219e.str

```
Αk
                Ak
                                 соон
             CH<sub>2</sub>
chain nodes : 11 13 14 15 17 18
ring nodes :
   1 2 3 4 5 6 7 8 9 10
chain bonds :
   4-13 4-14 9-15 11-17 17-18
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
    4-13 4-14 9-15 11-17 17-18
exact bonds :
   1-2 1-6 2-3 3-4 4-5
normalized bonds :
   5-6 5-7 6-10 7-8 8-9 9-10
isolated ring systems :
   containing 1 :
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:Atom 18:CLASS

: Unsaturated

Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

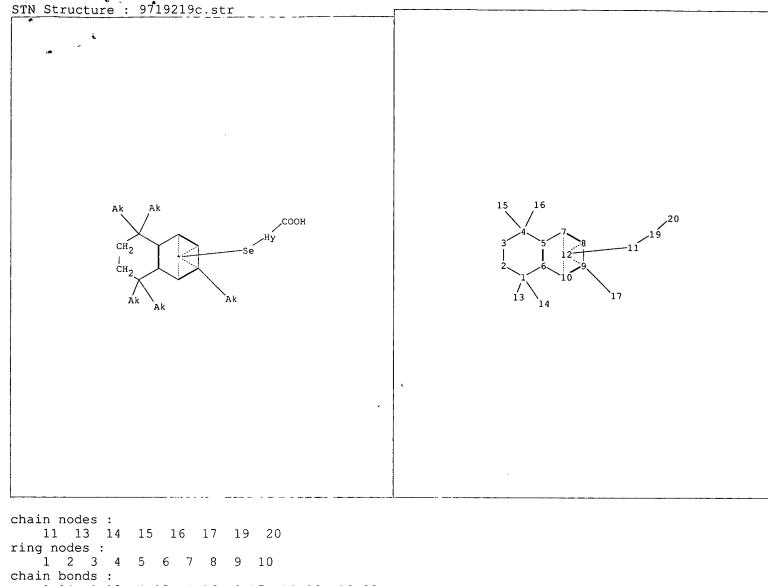
STN Structure: 9719219d.str

Match level :

17:

Generic attributes :

Saturation



```
ring nodes:
    1 2 3 4 5 6 7 8 9 10

chain bonds:
    1-14 1-13 4-15 4-16 9-17 11-19 19-20

ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds:
    1-14 1-13 4-15 4-16 9-17 11-19 19-20

exact bonds:
    1-2 1-6 2-3 3-4 4-5

normalized bonds:
    5-6 5-7 6-10 7-8 8-9 9-10

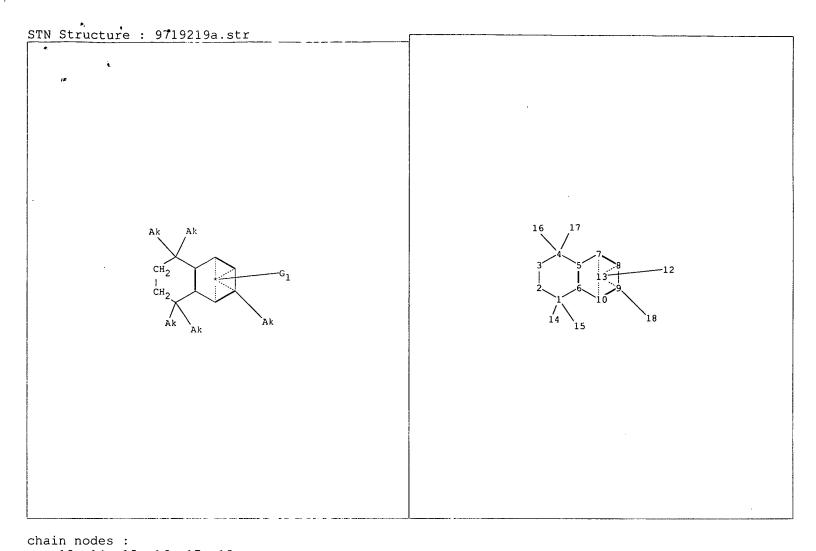
isolated ring systems:
    containing 1:
```

```
Match level :
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:Atom 20:CLASS Generic attributes :

19:

Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

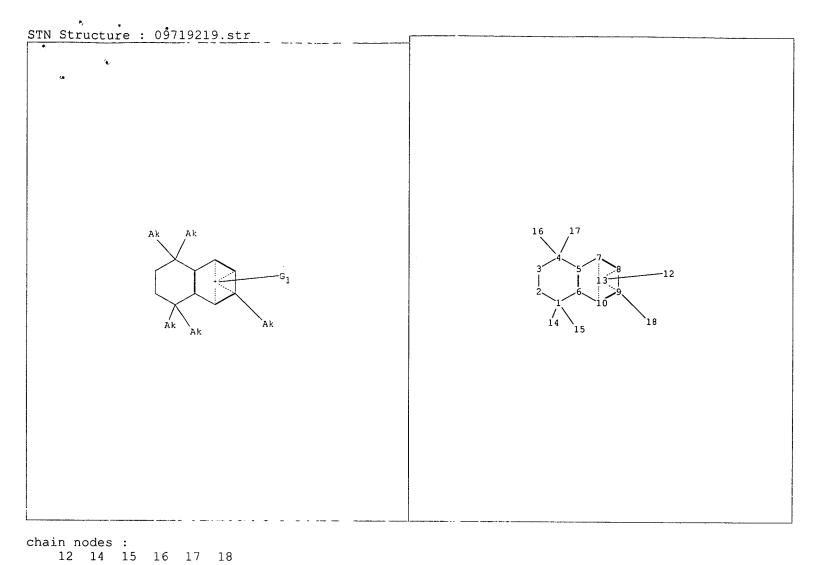


```
12 14 15 16 17 18
ring nodes :
   1 2 3 4
             5 6 7 8
chain bonds :
   1-15 1-14 4-16 4-17 9-18
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
   1-15 1-14 4-16 4-17 9-18
exact bonds :
   1-2 1-6 2-3 3-4 4-5
normalized bonds :
   5-6 5-7 6-10 7-8 8-9 9-10
isolated ring systems :
   containing 1 :
```

G1:0, S, Po, Se, Te

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS



```
ring nodes:

1 2 3 4 5 6 7 8 9 10

chain bonds:

1-15 1-14 4-16 4-17 9-18

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10

exact/norm bonds:

1-15 1-14 4-16 4-17 9-18

exact bonds:

1-2 1-6 2-3 3-4 4-5

normalized bonds:

5-6 5-7 6-10 7-8 8-9 9-10

isolated ring systems:

containing 1:
```

G1:O,S,Po,Se,Te

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

Connecting via Winsock to STN

Trying 3106016892...Open

Welcome to STN International! Enter x:x

LOGINID:ssspta1612BXR

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * Welcome to STN International

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Apr 23 PRE-1967 REFERENCES NOW SEARCHABLE IN CAPLUS AND CA

NEWS May 07 DGENE Reload

NEWS EXPRESS May 23 CURRENT WINDOWS VERSION IS V6.0a, CURRENT MACINTOSH VERSION IS V5.0C (ENG) AND V5.0JB (JP), AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2001 NEWS HOURS STN Operating Hours Plus Help Desk Availability General Internet Information NEWS INTER

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* * * * * * * * * * * * * * * STN Columbus

FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.15 0.15

FULL ESTIMATED COST

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15 JUN 2001 HIGHEST RN 341925-25-5 STRUCTURE FILE UPDATES: DICTIONARY FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5 TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See $\mbox{HELP SLIMIT}$ for details.

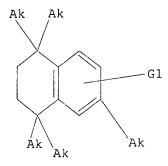
=>

Uploading 09719219.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS L1 STR



G1 O, S, Po, Se, Te

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 20:55:17 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 10238 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 198709 TO 210811

PROJECTED ANSWERS: 13 TO 395

L2 1 SEA SSS SAM L1

=> s 12 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:55:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 205394 TO ITERATE

100.0% PROCESSED 205394 ITERATIONS SEARCH TIME: 00.00.07

477 ANSWERS

L3 477 SEA SSS FUL L1

=> file ca

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 133.56 133.71

FULL ESTIMATED COST

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001
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FILE COVERS 1947 - 14 Jun 2001 VOL 134 ISS 26 FILE LAST UPDATED: 14 Jun 2001 (20010614/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

The CA file now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

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=> s 13

L4 133 L3

=> Uploading 9719219a.str

L5STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5

G1 O, S, Po, Se, Te

Structure attributes must be viewed using STN Express query preparation.

=> s 15

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 20:57:29 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 10238 TO ITERATE

9.8% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 198709 TO 210811 395

PROJECTED ANSWERS: 13 TO

L6 1 SEA SSS SAM L5

L7 1 L6

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL

Page 4

1 ANSWERS

ENTRY SESSION 0.31 135.26

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5 DICTIONARY FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> d his

(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 477 S L2 FULL

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001

L4 133 S L3

L5 STRUCTURE UPLOADED

S L5

FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001

L6 1 S L5

FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001 L7 1 S L6

FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001

=> d 16

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS

RN 191157-30-9 REGISTRY

CN 3-Pyridinecarboxylic acid, 6-[[(3-butoxy-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)carbonyl]oxy]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C25 H31 N O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> s 15 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:58:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 205394 TO ITERATE

100.0% PROCESSED 205394 ITERATIONS SEARCH TIME: 00.00.07

459 ANSWERS

L8 459 SEA SSS FUL L5

=> s 16 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 20:58:30 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 205394 TO ITERATE

100.0% PROCESSED 205394 ITERATIONS SEARCH TIME: 00.00.06

459 ANSWERS

L9 459 SEA SSS FUL L5

=> file req

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 269.86 405.12

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

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conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=>

Uploading 9719219c.str

L10 STRUCTURE UPLOADED

=> d 110

L10 HAS NO ANSWERS L10 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 110

SAMPLE SEARCH INITIATED 21:01:23 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2 TO 124

PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s 111 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:01:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 104 TO ITERATE

100.0% PROCESSED 104 ITERATIONS 1 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.01

L12 1 SEA SSS FUL L10

=> file ca

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 133.56 538.68

FULL ESTIMATED COST

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FILE COVERS 1947 - 14 Jun 2001 VOL 134 ISS 26 FILE LAST UPDATED: 14 Jun 2001 (20010614/ED)

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=> s 112

L13 2 L12

=> s 113 and bernardon, j?/au

58 BERNARDON, J?/AU

L14 1 L13 AND BERNARDON, J?/AU

=> d l14, ibib abs hitstr, 1

L14 ANSWER 1 OF 1 CA COPYRIGHT 2001 ACS ACCESSION NUMBER: 132:35910 CA

TITLE: Preparation of diaryl selenide compounds and their

use

in human or veterinary medicine and in cosmetics

Bernardon, Jean-Michel; Diaz, Philippe INVENTOR(S):

Galderma Research & Development, S.N.C., Fr. PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 81 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA | TENT | NO. | | KI | ND | DATE | | | A | PPLI | CATI | и ис | 0. | DATE | | | |
|---------|-------|------|------|-----|-----|------|------|------|------|------|------|-------|-----|------|------|-----|-----|
| WO | 9965 | 872 | | A | 1 | 1999 | 1223 | | W | 0 19 | 99-F | R138: | 9 | 1999 | 0611 | | |
| | W: | ΑE, | AL, | AM, | AT, | ΑU, | ΑZ, | BA, | BB, | BG, | BR, | BY, | CA, | CH, | CN, | CU, | CZ, |
| | | DE, | DK, | EE, | ES, | FI, | GB, | GD, | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, |
| | | JP, | KE, | KG, | ΚP, | KR, | ΚZ, | LC, | LK, | LR, | LS, | LT, | LU, | LV, | MD, | MG, | MK, |
| | | MN, | MW, | MX, | NO, | NΖ, | PL, | PT, | RO, | RU, | SD, | SE, | SG, | SI, | SK, | SL, | ТJ, |
| | | TM, | TR, | TT, | UA, | UG, | US, | UZ, | VN, | YU, | ZA, | ZW, | AM, | AZ, | BY, | KG, | ΚZ, |
| | | MD, | RU, | ТJ, | TM | | | | | | | | | | | | |
| | RW: | GH, | GM, | ΚE, | LS, | MW, | SD, | SL, | SZ, | ŪG, | ZW, | ΑT, | BE, | CH, | CY, | DE, | DK, |
| | | ES, | FI, | FR, | GB, | GR, | ΙE, | IT, | LU, | MC, | NL, | PT, | SE, | BF, | ВJ, | CF, | CG, |
| | | CI, | CM, | GΑ, | GN, | GW, | ML, | MR, | NE, | SN, | TD, | TG | | | | | |
| FR | 2779 | 720 | | А | 1 | 1999 | 1217 | | F | R 19 | 98-7 | 439 | | 1998 | 0612 | | |
| AU | 9940 | 491 | | A | 1 | 2000 | 0105 | | A | U 19 | 99-4 | 0491 | | 1999 | 0611 | | |
| EP | 1086 | 080 | | Α | 1 | 2001 | 0328 | | E | P 19 | 99-9 | 2372 | 3 | 1999 | 0611 | | |
| | R: | AT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | ΙΤ, | LI, | LU, | NL, | SE, | MC, | PT, |
| | | IE, | SI, | LT, | LV, | FI, | RO | | | | | | | | | | |
| NO | 2000 | 0063 | 37 | Α | | 2001 | 0212 | | N | 0 20 | 00-6 | 337 | | 2000 | 1212 | | |
| PRIORIT | Y APP | LN. | INFO | . : | | | | | FR 1 | 998- | 7439 | | Α | 1998 | 0612 | | |
| | | | | | | | | 1 | WO 1 | 999- | FR13 | 89 | W | 1999 | 0611 | | |
| OTHER S | OURCE | (S): | | | MAR | PAT | 132: | 3591 | 0 | | | | | | | | |

HER SOURCE(S):

GΙ

AΒ The invention concerns novel diaryl selenide compds. corresponding to I and their geometric and optical isomers and salts and the use thereof in pharmaceutical compns. in human or veterinary medicine (in the treatment of dermatol., rheumatic, cardiovascular and ophthalmol. pathologies in particular), or in cosmetic compns. In I, R1 = Me, CH2OR5 (R5 = H, lower alkyl, C(O)R10 (R10 = lower alkyl)), C(O)R6 (R6 = H, lower alkyl, OR12(R12 = H, lower alkyl, aryl, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl), NR'R'' (R'/R'' = H, lower alkyl,

aryl Page 9 possibly substituted, amino acid fragment; R' and R'' together with N form

a heterocycle)); Ar = R7-substituted benzene or pyridine diradical (R7 = H, halogen, lower alkyl, nitro, OR13 (R13 = H, lower alkyl), polyether radical, NR14R15 (R14/R15 = H, lower alkyl)), diradicals of furan, thiophene or thiazole; R2/R3 = H, tBu, 1-methylcyclohexyl, 1-adamantyl, OR8 (R8 = H, lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl), polyether radical, where at least one of R2 or R3 = tBu, 1-methylcyclohexyl, 1-adamantyl; R2 and R3 may together with an adjacent arom. ring form a satd. 5- or 6-membered ring possibly substituted by Me groups and/or possibly interrupted by O or S; R4 = H, halogen, lower alkyl, OR9 (R9 =

Н,

lower alkyl, aryl possibly substituted, aralkyl possibly substituted, monohydroxyalkyl, polyhydroxyalkyl, lower alkyl, (CH2)nCO2R16 (R16 = H, lower alkyl; n = 1-12), (CH2)nX (X = halogen)), polyether radical, C(0)R10. Although the method of prepn. is not claimed, 70 example

prepns.

are included. In a typical prepn., a haloarene (e.g. 2-bromo-5,6,7,8-tetrahydro-3,5,5,8,8-pentamethylnaphthalene) is successively reacted with tBuLi in THF, Se, and NaOH in EtOH to give a diselenide, which is cleaved with NaBH4 in EtOH to give the Na salt of an areneselenol, which is undergoes metathesis with IR1 or BrR1 (e.g. Et 4-iodobenzoate) in the presence of NiBr2py2 in EtOH to give I (e.g. Et 4-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)benzoate).

IT 252352-76-4, 6-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydronaphthalen-2-ylselenenyl)nicotinic acid

RL: RCT (Reactant)

(reactant; prepn. of diaryl selenide compds. and use in human or veterinary medicine and in cosmetics)

RN 252352-76-4 CA

CN 3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)seleno]-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

REFERENCE(S):

13

- (1) Allergan Inc; WO 9716422 A 1997 CA
- (2) Bernardon, J; WO 9822423 A 1998 CA
- (3) Boehm, M; Journal of Medicinal Chemistry 1995, V38, P3146 CA
- (4) Cird; WO 9220643 A 1992 CA
- (5) Cird, G; EP 0661258 A 1995 CA

ALL CITATIONS AVAILABLE IN THE RE FORMAT

(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001) FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001 STRUCTURE UPLOADED L11 S L1 L2 477 S L2 FULL L3 FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001 L4133 S L3 STRUCTURE UPLOADED L5 S L5 FILE 'REGISTRY' ENTERED AT 20:57:28 ON 17 JUN 2001 1 S L5 L6 FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001 1 S L6 L7FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001 $rac{1}{8}$ 459 S L5 FULL 459 S L6 FULL L9 FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001 STRUCTURE UPLOADED L10 0 S L10 L11 L12 1 S L11 FULL FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 2001 2 S L12 L13 1 S L13 AND BERNARDON, J?/AU L14 => s 113 not 114 1 L13 NOT L14 => s 115 and pd < july 1998 17097245 PD < JULY 1998 (PD<19980700) 0 L15 AND PD < JULY 1998 L16 => file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 7.88 546.56 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -0.56 -0.56CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 21:03:39 ON 17 JUN 2001

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STRUCTURE FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5 DICTIONARY FILE UPDATES: 15 JUN 2001 HIGHEST RN 341925-25-5

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> Uploading 9719219d.str

L17 STRUCTURE UPLOADED

=> d 117

L17 HAS NO ANSWERS L17 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 117

SAMPLE SEARCH INITIATED 21:03:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1872 TO ITERATE

53.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 34846 TO 40034 PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> s 118 full

0 ANSWERS

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:04:04 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 37574 TO ITERATE

100.0% PROCESSED 37574 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.02

O SEA SSS FUL L17 L19

=>

Uploading 9719219e.str

STRUCTURE UPLOADED L20

=> d 120

L20 HAS NO ANSWERS L20 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 120

SAMPLE SEARCH INITIATED 21:05:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1872 TO ITERATE

1000 ITERATIONS 53.4% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** 34846 TO 40034 PROJECTED ITERATIONS: O TO PROJECTED ANSWERS:

0 SEA SSS SAM L20

=> s 121 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

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6 ANSWERS

FULL SCREEN SEARCH COMPLETED - 37574 TO ITERATE

100.0% PROCESSED 37574 ITERATIONS

SEARCH TIME: 00.00.03

6 SEA SSS FUL L20

=> file hcaplus

L22

SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 813.99 267.43 FULL ESTIMATED COST SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) ENTRY SESSION 0.00 -0.56CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 21:05:16 ON 17 JUN 2001 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1947 - 17 Jun 2001 VOL 134 ISS 26 FILE LAST UPDATED: 15 Jun 2001 (20010615/ED)

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HCAplus now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

=> s 122

L23 16 L22

=> s 123 and bernardon, j?/au

61 BERNARDON, J?/AU L24 1 L23 AND BERNARDON, J?/AU

=> d 124, ibib abs hitstr, 1

L24 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2001 ACS ACCESSION NUMBER: 1995:995753 HCAPLUS

DOCUMENT NUMBER:

124:145647

TITLE:

Preparation of (tetrahydronaphthyloxy)benzoates and

analogs as cell proliferation inhibitors

INVENTOR(S):

Bernardon, Jean-Michel

PATENT ASSIGNEE(S):

Centre International de Recherches Dermatologiques

Galderma (C.I.R.D. Galderma), Fr.

SOURCE:

LANGUAGE:

Eur. Pat. Appl., 22 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| | PATENT NO |). | KIND | DATE | | | CATION NO |). - | DATE | | | |
|-------|------------|------------|-------------|------------|--------|--------|-----------|---------|-------|------|-----|------|
| | | | A1 | 19951102 | | | | 1 | 1995 | 0329 | | |
| | | | | 19980506 | | - CD | TO TO | т т | T 11 | MC | NIT | חיים |
| O.D. | R: A | T, BE, | CH, DE | E, DK, ES, | FK, G. | 3, GR, | 15, 11, | тт, | , LU, | MC, | ип, | P1, |
| SE | FR 271904 | 2 | 7\ 1 | 19951027 | | FR 19 | 91-5019 | | 1994 | 1426 | | |
| | FR 271904 | | | 19960531 | | IN IJ. | J4 J017 | | 1004 | 0420 | | |
| | AT 165807 | | | | | ልጥ 104 | 95-40070 | 1 | 1995 | 0329 | | |
| | EC 211022 |) <i>C</i> | и. З | 19981001 | | FC 10 | 95-40070. | 1 | | | | |
| | ZA 950297 | | | | | 7A 19 | 95-2974 | 1 | 1995 | 0323 | | |
| | AU 951651 | | | | | | 95-16512 | | | | | |
| | AU 931031 | . 4 | R2 | 19960502 | | no is | JJ 10312 | | 1000 | 0110 | | |
| | NO 950154 | , | Δ | 19951027 | | NO 19 | 95-1545 | | 1995 | 0424 | | |
| | CA 214780 | | | 19951027 | | | | | | | | |
| | FI 950196 | | | | | | 95-1967 | | | | | |
| | JP 081698 | | | 19960702 | | | | | | | | _ |
| | HU 74014 | , , , | Δ2 | 19961028 | | | 95-1167 | | | | | |
| | BR 950161 | 2 | Δ | | | | 95-1612 | | | | | |
| | RU 214147 | 71 | C1 | 19991120 | | | 95-10668 | | | | | |
| | PL 179902 |) | R1 | 20001130 | | | | | 1995 | | | |
| | US 576661 | | | 19980616 | | | | | 1995 | 0426 | | |
| | US 601556 | 59 | A | 20000118 | | | 97-97198 | | | | | |
| | US 616281 | | | | | | 98-15072 | | | | | |
| | US 615678 | 38 | A | 20001205 | , | US 19 | 99-36987 | 5 | 1999 | 0809 | | |
| PRIOF | RITY APPLN | | | 20001200 | FR | 1994- | 5019 | Α | 1994 | 0426 | • | |
| | | | | | US | 1995- | 429096 | A1 | 1995 | 0426 | | |
| | | | | | | | 971983 | | | | | |

OTHER SOURCE(S):

MARPAT 124:145647

GΙ

Title compds. [I; R = ZR1; R1 = (un)substituted Ph, -heterocyclyl; R2 = AB Η, halo, alkyl, etc.; Z = 0, SOO-2, (alkyl)imino; Z1,Z2 = 0, SOO-2, (di)(alkyl)methylene] were prepd. as cell proliferation inhibitors (no data). Thus, 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthol was etherified by 4-IC6H4CO2Me and the product sapond. to give title compd.

IT

173156-90-6P 173156-98-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (tetrahydronaphthyloxy)benzoates and analogs as cell proliferation inhibitors)

173156-90-6 HCAPLUS RN

2-Thiophenecarboxylic acid, 5-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-CN naphthalenyl)thio] - (9CI) (CA INDEX NAME)

RN 173156-98-4 HCAPLUS

3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2naphthalenyl)thio]- (9CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 20:54:36 ON 17 JUN 2001)

FILE 'REGISTRY' ENTERED AT 20:54:45 ON 17 JUN 2001

STRUCTURE UPLOADED L1

L21 S L1

477 S L2 FULL L3

FILE 'CA' ENTERED AT 20:55:37 ON 17 JUN 2001

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133 S L3
L4
                STRUCTURE UPLOADED
L5
                S L5
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              1 S L5
L6
     FILE 'CA' ENTERED AT 20:57:30 ON 17 JUN 2001
L7
              1 S L6
     FILE 'REGISTRY' ENTERED AT 20:57:35 ON 17 JUN 2001
            459 S L5 FULL
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            459 S L6 FULL
L9
     FILE 'REGISTRY' ENTERED AT 21:01:02 ON 17 JUN 2001
               STRUCTURE UPLOADED
L10
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     FILE 'CA' ENTERED AT 21:01:38 ON 17 JUN 2001
              2 S L12
L13
              1 S L13 AND BERNARDON, J?/AU
L14
L15
              1 S L13 NOT L14
              0 S L15 AND PD < JULY 1998
L16
     FILE 'REGISTRY' ENTERED AT 21:03:39 ON 17 JUN 2001
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L17
              0 S L17
L18
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L19
                STRUCTURE UPLOADED
L20
              0 S L20
L21
              6 S L21 FULL
L22
     FILE 'HCAPLUS' ENTERED AT 21:05:16 ON 17 JUN 2001
L23
             16 S L22
              1 S L23 AND BERNARDON, J?/AU
L24
=> s 123 and pd < july 1998
      17383507 PD < JULY 1998
                  (PD<19980700)
             7 L23 AND PD < JULY 1998
L25
\Rightarrow d 125, ibib abs fhitstr, 1-7
L25 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2001 ACS
                          1998:728106 HCAPLUS
ACCESSION NUMBER:
                          130:104932
DOCUMENT NUMBER:
TITLE:
                          ET-1 expression and growth inhibition of prostate
                          cancer cells: a retinoid target with novel
specificity
                          Hsu, Ju-Yu; Pfahl, Magnus
AUTHOR(S):
                          Sidney Kimmel Cancer Center, San Diego, CA, 92121,
CORPORATE SOURCE:
USA
                          Cancer Res. (1998), 58(21), 4817-4822
SOURCE:
```

Page 17

CODEN: CNREA8; ISSN: 0008-5472

AACR Subscription Office PUBLISHER:

DOCUMENT TYPE: Journal English LANGUAGE:

Endothelin-1 (ET-1) is not only a potent vasoconstrictor but also serves as an important growth stimulator in various cancers, including breast, cervical, pancreatic, and prostate cancer. This suggests that blockage

of ET-1 prodn. may suppress tumor growth and possibly metastasis. The authors obsd. that certain synthetic retinoids and all-trans-retinoic acid

can repress LNCaP prostate cancer cell growth in vitro. In addn., these retinoid compds. counteracted exogenous ET-1-induced growth stimulation. Retinoid-dependent growth retardation of LNCaP cells coincided with suppression of ET-1 gene expression to a level undetectable by reverse transcription-PCR. Contrarily, the androgen-insensitive DU145 cells were refractory to retinoid treatment. To investigate the underlying mechanisms of the cell-specific response to retinoids, the authors transfected ET-1 promoter constructs contg. wild-type or mutated AP-1 or GATA-2 site into prostate cancer cells. Distinct regulations of ET-1 promoter activity were found; in LNCaP cells, both binding sites are essential for optimal promoter activation, whereas in DU145 cells, addnl. promoter sequences and/or transcriptional factors seem to be involved. Furthermore, several anti-AP-1 selective retinoids failed to repress ET-1 promoter activity and to exhibit a cell growth-inhibitory effect on LNCaP cells, suggesting that different retinoid structural configurations are required for the inhibition of an AP-1 complex vs. an AP-1/GATA-2

complex. 173156-98-4, CD 2809

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(endothelin 1 expression and growth inhibition of prostate cancer

cells

response to retinoids in relation to AP-1 and GATA-2 sites in endothelin 1 promoter)

173156-98-4 HCAPLUS RN

3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2naphthalenyl)thio]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

REFERENCE(S):

(3) Baley, P; J Clin Invest 1990, V85, P1320 HCAPLUS

(4) Benatti, L; J Clin Invest 1993, V91, P1149

HCAPLUS

(5) Blutt, S; Endocrinology 1997, V138, P1491 HCAPLUS

(6) Dawson, M; Cancer Res 1995, V55, P4446 HCAPLUS

(7) Dawson, M; J Med Chem 1995, V38, P3368 HCAPLUS ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2001 ACS ACCESSION NUMBER: 1998:206286 HCAPLUS

DOCUMENT NUMBER: 128:317589

TITLE: Inhibition of the 1,25-dihydroxyvitamin D3-induced

increase in vitamin D receptor (VDR) levels and

binding of VDR-retinoid X receptor (RXR) to a direct

repeat (DR)-3 type response element by an

RXR-specific

ligand in human keratinocyte cultures

AUTHOR(S): Jensen, Tina J.; Henriksen, Linda O.; Solvsten,

Henrik; Kragballe, Knud

CORPORATE SOURCE: DEPARTMENT OF DERMATOLOGY, MARSELISHORG HOSPITAL,

AARHUS C, DK-8000, Den.

SOURCE: Biochem. Pharmacol. (1998), 55(6), 767-773

CODEN: BCPCA6; ISSN: 0006-2952

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

The biol. active form of vitamin D, 1,25-dihydroxyvitamin D3 (1,25(OH)2D3), mediates most of its actions through the intracellular vitamin D receptor (VDR). VDR binds to vitamin D responsive elements (VDREs) in the promoter region of responsive genes and regulates transcription. Usually the VDREs consist of a direct repeat of two hexanucleotides spaced by three nucleotides (DR-3), to which VDR preferentially binds as a heterodimer with the retinoid X receptor (RXR). In the present study, we examd. the effect of 1,25(OH)2D3 and a specific ligand for RXR, CD2809, on VDR and RXR levels in cultured human keratinocytes and on the binding of RXR-VDR to a DR-3 type response element. Incubation with 1,25(OH)2D3 increased VDR levels as detd. by Western blotting, increased VDR-RXR binding to a DR-3 type response element as detd. by the electromobility shift assay (EMSA), and induced the 25-OH-D3 24-hydroxylase (24-hydroxylase) gene, contg. a DR-3 type response element. CD2809 caused a slight decrease in RXR.alpha. levels, but had no effect on VDR levels. Addn. of both CD2809 and 1,25(OH)2D3 decreased VDR levels as well as the VDR-RXR binding levels to the DR-3 type response element, compared to 1,25(OH)2D3 alone. In conclusion, an RXR-specific ligand interferes with the 1,25(OH)2D3-induced stimulation of

VDR levels and VDR-RXR binding to DNA in keratinocyte cultures. It is therefore possible that RXR-specific ligands may counteract certain biol. actions of vitamin D3-.

IT 173156-98-4, CD2809

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(dihydroxyvitamin D3 effect on VDR and RXR.alpha. levels and the binding of VDR-RXR to a direct repeat (DR)-3 type response element in relation to costimulatory effects of the RXR-specific ligand CD2809)

RN 173156-98-4 HCAPLUS

CN 3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)thio]-(9CI) (CA INDEX NAME)

L25 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2001 ACS 1998:175698 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

128:213396

TITLE:

Use of retinoids for the preparation of a medicament for treating disorders related to VEGF overexpression

INVENTOR(S):

Vega, Barbara; Michel, Serge; Ladoux, Annie; Frelin,

Christian

PATENT ASSIGNEE(S):

Centre International de Recherches Dermatologiques

Galderma, (Cird Galderma), Fr. Eur. Pat. Appl., 9 pp.

SOURCE:

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------|--------|-------------|-------------------------|-----------------|
| EP 826368 | A1 | 19980304 | | 19970827 < |
| • | CH, DE | , DK, ES, I | FR, GB, GR, IT, LI, LU, | NL, SE, MC, PT, |
| IE, FI | | | | |
| FR 2752734 | A1 | 19980306 | FR 1996-10685 | 19960902 < |
| FR 2752734 | В1 | 19981106 | | |
| CA 2213690 | AA | 19980302 | CA 1997-2213690 | 19970829 < |
| AU 9736090 . | Al | 19980305 | AU 1997-36090 | 19970829 < |
| AU 712750 | B2 | 19991118 | | |
| BR 9702808 | А | 19990105 | BR 1997-2808 | 19970829 |
| JP 10087481 | A2 | 19980407 | JP 1997-236308 | 19970901 < |
| JP 3107775 | В2 | 20001113 | | |
| US 6001885 | Α | 19991214 | US 1997-921511 | 19970902 |
| PRIORITY APPLN. INFO. | . : | | FR 1996-10685 A | 19960902 |

Retinoids, particularly anti-AP1 are used for the prepn. of a medicament AB for treating disorders related to VEGF (vascular endothelial growth factor) overexpression, e.g. psoriasis and Kaposi syndrome. Thus, 6-[3-(1-adamantyl)-4-methoxyphenyl]2-naphthoic acid at 10-8 M concn. inhibited the expression of VEGF in cultured keratinocytes by 58% as compared with glyceraldehyde phosphate dehydrogenase.

ΙT 204332-26-3

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(use of retinoids for prepn. of medicament for treating disorders related to VEGF overexpression)

RN 204332-26-3 HCAPLUS

3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2naphthalenyl)sulfonyl]- (9CI) (CA INDEX NAME)

L25 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2001 ACS ACCESSION NUMBER: 1997:549073 HCAPLUS

DOCUMENT NUMBER: 127:243238

TITLE: Effects of vitamin D3 on keratinocyte proliferation

and differentiation in vitro. Modulation by ligands

for retinoic acid and retinoid X receptors

AUTHOR(S): Sorensen, S.; Solvsten, H.; Politi, Y.; Kragballe,

Knut

CORPORATE SOURCE: Marselisborg Hospital, University Aarhus, Aarhus,

DK-8000, Den.

SOURCE: Skin Pharmacol. (1997), 10(3), 144-152

CODEN: SKPHEU; ISSN: 1011-0283

PUBLISHER: Karger
DOCUMENT TYPE: Journal
LANGUAGE: English

The antiproliferative and prodifferentiating effects of 1,25-dihydroxyvitamin D3 (1,25(OH)2D3) on normal human keratinocyte cultures were investigated after incubation for 4 days with the ligands all-trans-retinoic acid (all-trans RA), CD2809, 9-cis-retinoic acid (9-cis-RA), and triiodothyronine (T3). Proliferation was measured by the dimethylthiazolyl-diphenyl-tetrazolium-bromide assay and differentiation was detd. in the same culture with a cell ELISA for transglutaminase type I. All-trans RA, 9-cis-RA, and CD2809 had a slight stimulatory effect on proliferation. In combination with 1,25(OH)2D3, all retinoids partially counteracted the antiproliferative effect of 1,25(OH)2D3. The differentiation was inhibited dose-dependently by all-trans RA, 9-cis-RA, and CD2809. In combination with 1,25(OH)2D3 resulting in a net inhibition

differentiation. T3 alone or in combination with 1,25(OH)2D3 had no effect on proliferation or differentiation. Ligand-dependent heterodimer formation between the vitamin D receptor and retinoid receptors may not

important for the combined effects of 1,25(OH)2D3 and retinoids on keratinocyte proliferation and differentiation in vitro.

IT 173156-98-4, CD 2809

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RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(effects of vitamin D3 on keratinocyte proliferation and differentiation, modulation by ligands for retinoic acid and retinoid

receptors)
RN 173156-98-4 HCAPLUS
CN 3-Pyridinecarboxylic acid,
6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-

naphthalenyl)thio] - (9CI) (CA INDEX NAME)

L25 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2001 ACS 1997:403183 HCAPLUS ACCESSION NUMBER:

127:17489 DOCUMENT NUMBER:

Preparation of tetrahydronaphthylthiobenzoates and TITLE:

analogs as retinoid X receptor agonists

Beard, Richard L.; Colon, Diana F.; Chandraratna, INVENTOR(S):

Roshantha A. Allergan, USA PATENT ASSIGNEE(S):

PCT Int. Appl., 49 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PA' | TENT 1 | NO. | | KII | ND | DATE | | | A. | PPLI | CATI | N NC | ο. | DATE | | | |
|---------|--------|-------|------|-----|-----|------|------|------|------|------|---------------|------|-----|------|------|-----|-----|
| | | | | | | | | | _ | | - - | | | | | | |
| WO | 9716 | 422 | | A. | 1 | 1997 | 0509 | | W | 0 19 | 96 - U | S172 | 95 | 1996 | 1029 | < | |
| | W: | | | | | | | | | | | | | CZ, | | | |
| | | | | | | | | | | | | | | ΚZ, | | | |
| | | | | | | | | | | | | | | PT, | | | |
| | | SE, | SG, | SI, | SK, | ТJ, | TM, | TR, | TT, | UA, | UG, | UZ, | VN, | AM, | AZ, | BY, | KG, |
| | | | MD, | | | | | | | | | | | | | | |
| | R₩: | | | | | | | | | | | | | FI, | | | GR, |
| | | ΙE, | | | | | | | | | | | | CM, | | | |
| AU | 9675 | 985 | | A. | 1 | 1997 | 0522 | | A. | U 19 | 96-7: | 5985 | | 1994 | 1029 | < | |
| US | 5672 | 710 | | А | | 1997 | 0930 | | | | | | - | 1995 | | < | |
| PRIORIT | Y APP | LN. | INFO | . : | | | | | US 1 | 995- | 5529 | 65 | | 1995 | 1101 | | |
| | | | | | | | | 1 | WO 1 | 996- | US17 | 295 | | 1996 | 1029 | | |
| OTHER C | OHIDOE | 101 . | | | MΔR | PAT | 127. | 1748 | 9 | | | | | | | | |

OTHER SOURCE(S):

MARPAT 127:17489

GΙ

$$R^1$$
 R^2
 R^3
 R^1
 R^2
 R^2
 R^3
 R^3

Title compds. [I; R = SOO-2ZAB; A = bond, alk(en)ylene, alkynylene; B =AB Η, Page 22

CH2OH, alkoxycarbonyl, etc.; R1 = H or alkyl; R2 = 1-3 substituents selected from H, halo, alkyl, alkoxy, etc.; R3 = 1-4 substituents selected

from H, F, alkyl; X = O, S, (alkyl)imino, CH2, etc.; Z = (un) substituted phenylene, -heteroarylene] were prepd. Thus, 5,6,7,8-tetrahydro-5,5,8,8tetramethylnaphthalene-2-thiol was thioetherified by 4-IC6H4CO2Et to give title compd. II. Data for biol. activity of I were given.

IT 190596-59-9P

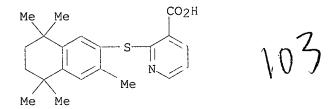
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of tetrahydronaphthylthiobenzoates and analogs as retinoid Xreceptor agonists)

190596-59-9 HCAPLUS RN

3-Pyridinecarboxylic acid, CN

2-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2naphthalenyl)thio]- (9CI) (CA INDEX NAME)



L25 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2001 ACS 1996:483612 HCAPLUS ACCESSION NUMBER:

125:131667 DOCUMENT NUMBER:

Synthesis and Structure-Activity Relationships of TITLE: Retinoid X Receptor Selective Diaryl Sulfide Analogs

of Retinoic Acid

Beard, Richard L.; Colon, Diana F.; Song, Tae K.; AUTHOR(S):

Davies, Peter J. A.; Kochhar, Devendra M.;

Chandraratna, Roshantha A. S.

Department of Chemistry, Allergan Incorporated, CORPORATE SOURCE:

Irvine, CA, 92715-1599, USA

J. Med. Chem. (1996), 39(18), 3556-3563 SOURCE:

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal English LANGUAGE:

Retinoids exert their biol. effects by binding to and activating nuclear receptors that interact with responsive elements on DNA to promote gene transcription. There are two families of retinoid receptors, the retinoic

acid receptor (RAR) family and the retinoid X receptor (RXR) family, which

are each further divided into three subclasses: RAR.alpha.,.beta.,.gamma. and RXR.alpha., .beta., .gamma.. Herein we describe the synthesis and structure-activity relationships SAR of a new series of diaryl sulfide retinoid analogs that specifically bind and transactivate the RXRs. Furthermore, the sulfoxide and sulfone derivs. of these analogs are partial agonists which activate the RXRs only at high concns. Thus,

these Page 23

compds. possess a potential site of metabolic deactivation and may have less prolonged systemic effects than other compds. with arotinoid-like structures. We show also that these compds. have activity in nontransfected cells as demonstrated by their ability to induce TGase activity in HL-60 cells. Finally, we corroborate our earlier report that RXR-specific agonists may possess reduced teratogenic toxicity compared

to

RAR-specific agonists since these compds. are much less potent inhibitors of chondrogenesis than RAR-specific agonists such as TTNPB.

173156-98-4P IT

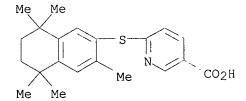
> RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and structure-activity relationships of retinoid x receptor selective diaryl sulfide analogs of retinoic acid)

173156-98-4 HCAPLUS RN

3-Pyridinecarboxylic acid,

6-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2naphthalenyl)thio]- (9CI) (CA INDEX NAME)





L25 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2001 ACS ACCESSION NUMBER: 1995:995753 HCAPLUS

124:145647 DOCUMENT NUMBER:

Preparation of (tetrahydronaphthyloxy)benzoates and TITLE:

analogs as cell proliferation inhibitors

Bernardon, Jean-Michel INVENTOR(S):

Centre International de Recherches Dermatologiques PATENT ASSIGNEE(S):

Galderma (C.I.R.D. Galderma), Fr.

Eur. Pat. Appl., 22 pp. SOURCE:

CODEN: EPXXDW

Patent DOCUMENT TYPE: French LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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|-----|------------------------------------|---------------|----------------------------------|----------------------------------|------------------------|
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| | R: AT, BE, | | | GB, GR, IE, IT, LI | , LU, MC, NL, PT, |
| | R 2719043 | A1 | 19951027 | FR 1994-5019 | 19940426 < |
| A | R 2719043 F 165807 S 2119326 | B1 E T3 | 19960531 19980515 19981001 | AT 1995-400701 ES 1995-400701 | 19950329 < 19950329 |

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PRIORITY APPLN. INFO.:
                                          US 1995-429096
                                                             A1 19950426
                                                             A2 19971117
                                          US 1997-971983
                          MARPAT 124:145647
OTHER SOURCE(S):
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AB Title compds. [I; R = ZR1; R1 = (un)substituted Ph, -heterocyclyl; R2 = H, halo, alkyl, etc.; Z = O, SOO-2, (alkyl)imino; Z1, Z2 = O, SOO-2, (di)(alkyl)methylene] were prepd. as cell proliferation inhibitors (no data). Thus, 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthol was etherified by 4-IC6H4CO2Me and the product sapond. to give title compd. II.

IT 173156-90-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (tetrahydronaphthyloxy)benzoates and analogs as cell proliferation inhibitors)

RN 173156-90-6 HCAPLUS

CN 2-Thiophenecarboxylic acid, 5-[(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)thio]- (9CI) (CA INDEX NAME)

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